Supplementary Material

Optical multisensor system based on lanthanide(III) complexes as near-infrared light sources for analysis of milk

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Lanthanide complexes were chosen based on the following reasons:

(a) Predictability of NIR emission energy. The emission wavelength of Ln(III) complexes remains the same when the ligand environment is changed because luminescence is a result of intrametal transitions, information about which is very well known.

(b) The ytterbium and neodymium complexes are the most popular NIR emitters for working with biological objects, because their photoemission is within the transparency window of most biological objects (ca. 700 to ca. 1100 nm). Additionally, the luminescence band of ytterbium at ca. 1000 nm partially overlaps with the absorption band of water, which allows a comparative assessment of the water content in different samples.

(c) In contrast to phosphorescence of d-metals complexes, the luminescence of Ln(III) is not sensitive to oxygen that allows to work without sample degassing.

(d) Tris(beta-diketonate) heteroleptic Ln(III) complexes are air-, moister- and photostable. The synthetic procedure is very well known and lead to preparing of the product with high yield.

Low quantum yield of NIR photoemission is ordinary situation due to Jörtner's energy gap law (the non-radiative rate constant increases exponentially with the decrease of the energy gap between the ground and the excited state) and all NIR emitters suffer of weak emission intensity.

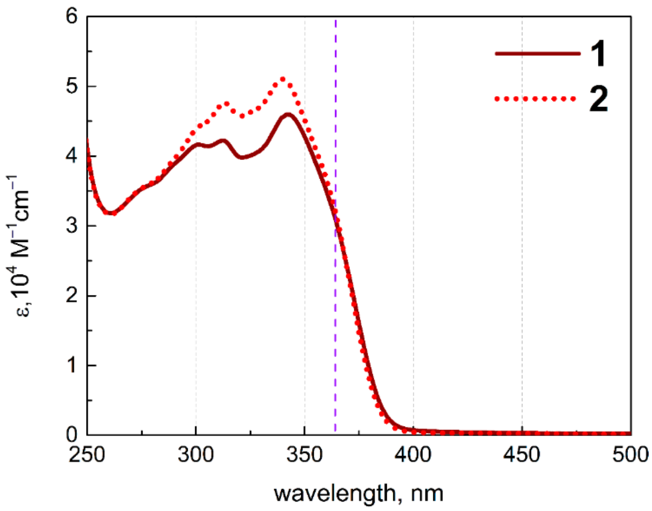

Figure S1. Solid-state emission of complexes **1** and **2 in UV-Vis region,** λ_{exct} = 365 nm, room temperature.

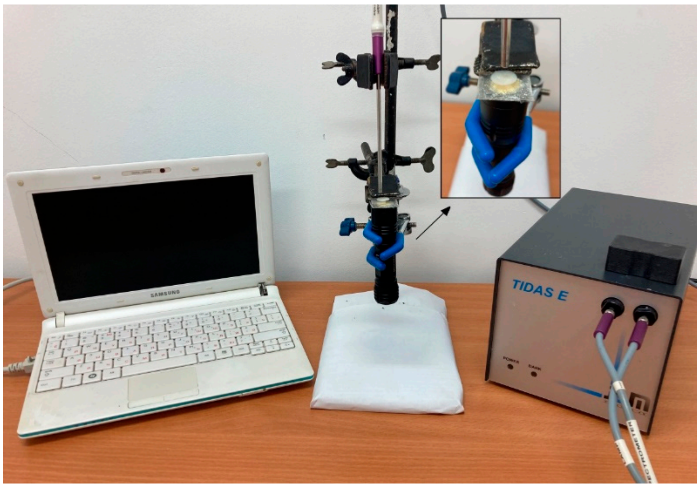

Figure S2. The photo of the OMS prototype-2.

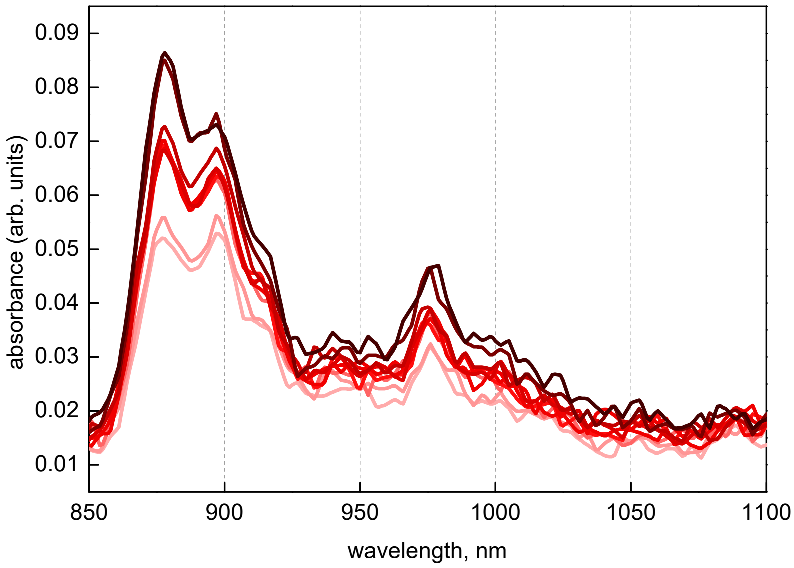

Figure S3. The raw NIR spectra of the milk samples (F2-series) with varying fat content in absorbance mode (red gradient indicates an increase in the concentration of fat).

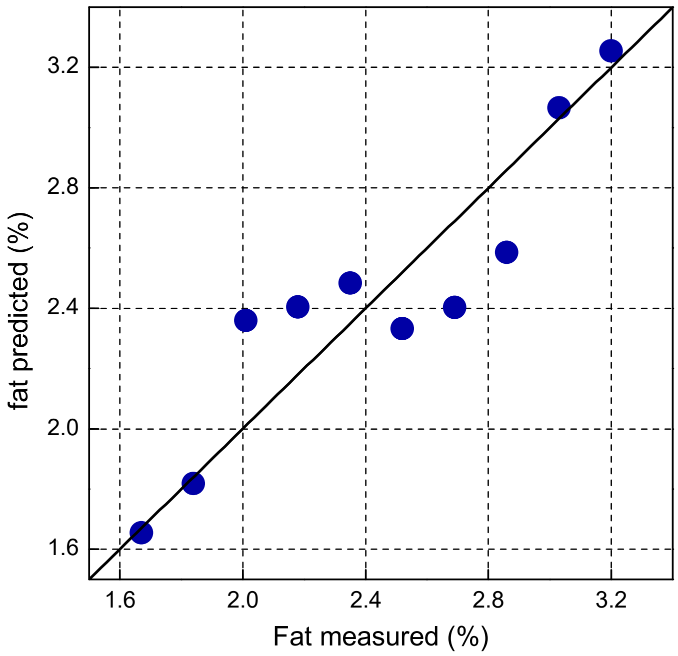

Figure S4. Predicted versus measured plot for quantification of fat (F2-series) for the full-spectrum PLS regression model (850–1100 nm) in absorbance mode. Blue circles indicate full cross-validation results.

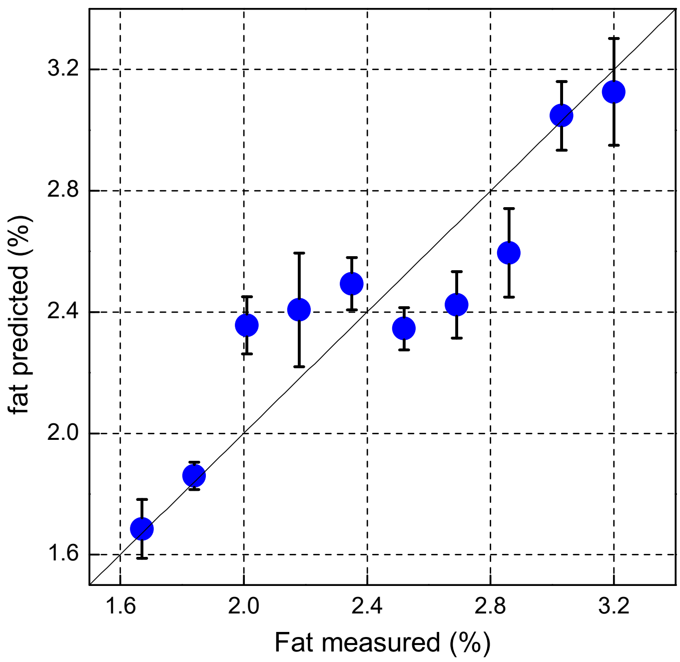

Figure S5. Predicted versus measured predicted plot for quantification of fat (F2-series) for the full-spectrum PLS regression model (850–1100 nm) in absorbance mode. Blue circles represent an average of five repeats and the error bars represent the standard deviation.